

Systems & Control *Transactions*

Volume 4

Proceedings of the 35th

European Symposium on Computer Aided Process Engineering

ESCAPE 35



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Systems & Control Transactions

Vol 4

Proceedings of the 35th European Symposium
on Computer Aided Process Engineering
ESCAPE 35

July 6–9, 2025
Ghent, Belgium



PSEcommunity.org

PSE Press • Hamilton • Notre Dame

Systems & Control Transactions, Volume 4
PSE Press
Hamilton, Ontario, Canada

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Living Archive for Process Systems Engineering (LAPSE) Archive ID: LAPSE:2025.0150
Digital Object Identifier (DOI): 10.69997/sct.173479

Library and Archives Canada Catalogue

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Electronic Book
ISBN (Volume 4) 978-1-7779403-3-1
ISSN (Series): 2818-4734

10 9 8 7 6 5 4 3 2 1

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Typeset in Inter

Suggested Citation for Individual Articles

Student MC, Supervisor QR. Title of the article. *Systems & Control Transactions* 4:startpage-endpage (2025). <https://doi.org/10.69997/sct.restofarticledoi>

Suggested Citation for Entire Proceedings

Van Impe JFM, Léonard G, Bhonsale SS, Polańska ME, and Logist F (eds). Proceedings of the 35th European Symposium on Computer Aided Process Engineering, Ghent, Belgium, July 6-9 (2025). ISBN: 978-1-7779403-3-1

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Introduction

Jan Van Impe, Grégoire Léonard, Satyajeet Sheetal Bhonsale, Monika Polanska, and Filip Logist (eds)

The 35th European Symposium on Computer Aided Process Engineering (ESCAPE|35) was held at KU Leuven/Campus Gent, Belgium, July 6–9, 2025. Continuing a tradition that began in 1991 under the auspices of the EFCE Working Party on Computer Aided Process Engineering (CAPE), the ESCAPE series stands as a premier annual event for the global Process Systems Engineering (PSE) community. ESCAPE returned to Belgium for the second time - following the 1998 edition in Bruges - and took place as part of KU Leuven's 600th anniversary celebrations. The 35th edition was organised jointly by KU Leuven/BioTeC+ and University of Liège/PEP.

The 2025 conference embraced the theme "Closing the Loop 2.0", underscoring the evolving role of PSE in enabling a circular economy. The program highlighted both core process engineering disciplines – such as modeling, control, design, and optimization – and cutting-edge approaches involving artificial intelligence, machine learning, and quantum computing, applied across diverse sectors including energy, chemicals, biotechnology, and advanced materials.

ESCAPE|35 received 673 abstract submissions, of which 563 were invited for a 5-to-8-page full paper or a 2-page short paper after a first review round. Upon rigorous re-review of all papers submitted, 423 full paper contributions have been published in full open access (and LAPSE and DOI indexed) by PSE Press as a separate volume of the *Systems & Control Transactions* series. Another 140 contributions have been made available as two pages short papers published by EUROSIS-ETI.

The scientific contributions were organized into thematic sessions, poster presentations, workshops, and demonstrations, within ten thematic tracks:

- T01: Modelling and Simulation
- T02: Sustainable Product Development and Process Design
- T03: Large Scale Design and Planning/Scheduling
- T04: Model-Based Optimisation and Advanced Control
- T05: Concepts, Methods and Tools
- T06: Digitalization and AI
- T07: CAPEing with Societal Challenges (Green Deal, Energy Transition, ...)
- T08: CAPE Education and Knowledge Transfer
- T09: PSE4Food and Biochemical (*new in 2025*)
- T10: PSE4BioMedical and (Bio)Pharma (*new in 2025*)

Tracks T09 and T10 were introduced in this year's edition to broaden the application scope of PSE methods in food, biochemical, (bio)pharma and biomedical systems - fields of increasing relevance to the community.

We extend our sincere thanks to all authors, reviewers, topic coordinators, plenary and keynote speakers, and members of the Scientific and Organizing Committees. We gratefully acknowledge KU Leuven and University of Liège for their support and express our heartfelt appreciation to our numerous sponsors. This edition also marks the inaugural collaboration with PSE Press as the official publisher of the ESCAPE proceedings (full papers volume) - a milestone in promoting high-quality, open access dissemination of PSE research. Many thanks to EUROSIS-ETI as well for publishing the short papers volume, ISBN indexed.

We hope these volumes capture the scientific excellence, collaborative spirit, and forward-looking vision that defined ESCAPE|35 and continue to serve as a valuable reference for researchers and practitioners in the years ahead.

ESCAPE|35 - European Symposium on Computer Aided Process Engineering

Ghent, Belgium. 6-9 July 2025

Peer Review Policy

TERMINOLOGY

- **Conference Paper:** This is a peer-reviewed research paper describing an **original** research contribution and published in the conference proceedings.

APPLICATION

- All conference papers are subject to peer review.

PUBLICATIONS

- All conference papers which have passed peer review and have been accepted by the conference chairs will be published in the conference proceedings.

PEER REVIEW PROCESS

Initial Screening

The conference chairs will screen the initial submissions (one-page abstracts) of contributed papers. At their option, chairs may choose to reject these submissions for any reason, but the primary reasons for rejection at this stage are (a) subject does not match conference themes and topics; (b) in appropriate, unprofessional, unethical, or dishonest material; (c) duplicate submissions; (d) abandoned submissions; (e) multiple submissions from same presenter; (f) obvious poor quality; (g) reasonable suspicion of machine-generated text; (h) need to limit acceptances because of conference space constraints. Chairs may also transfer papers between sessions at this stage.

Conference chairs will then invite authors of the one-page abstracts that have passed the initial screening to submit a conference paper for peer review.

Conference Paper Peer Review

Conference chairs act as editors. They will assign peer reviewers to assess the quality of the conference papers and manage the peer review process for each paper. Peer reviewers are generally selected from the International Scientific Committee who are scientists, engineers, or researchers with technical expertise in the conference topic. Peer reviewers must be considered technical experts in their field, hold a PhD, and have published peer reviewed scientific works previously. Each work must be reviewed by a minimum of two peer-reviewers.

A “single-blind” peer review system is used, in which the peer reviewers have access to the identities of the authors, but the authors are never given the identities of the peer reviewers. This is consistent with most journal peer-review procedures in our field.

Peer reviewers will be given a set of quality criteria that may include scientific and technical quality, quality of writing, originality and novelty, appropriateness for the conference topic and theme, interest to the community, and other factors of merit. Peer reviewers are expected to be rigorous and critical in their technical assessments and adhere to the highest standards in the field in order to ensure high quality. Peer reviewers are asked to comment on their assigned conference papers and issue a recommendation to the conference chairs based on this quality criteria. Reviewers may recommend one of the following:

- **Accept Paper.** No technical changes are necessary before publication. Only typographical, spelling, grammar, or other minor changes are necessary which do not require technical review.
- **Accept Paper with Minor Revisions.** Some minor technical issues need to be addressed either through technical changes to the manuscript or through rebuttal to reviewer comments. The reviewer does not believe the issues are significant enough to require additional technical review by the reviewers. The reviewer has provided enough commentary such that the editor can decide if the minor issues have been addressed in a future revision.
- **Revise Paper with Re-Review.** Major technical issues need to be addressed either through technical changes

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The conference chairs are responsible for making the final decision on each paper and may require several rounds of author changes if necessary to meet quality standards. Conference chairs are not required to follow the recommendations of the peer reviewers in making these decisions. It is possible that conference chairs will choose to not accept some papers that still pass through rigorous technical peer review, especially when limited by available space or when papers do not sufficiently promote conference objectives. Conference chairs may also transfer papers between sessions as desired.

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The chairs and peer reviewers must ensure they do not have a conflict of interest that may bias their decisions, such as ensuring that authors are at “arm’s length” and have no financial conflicts of interest. Peer reviewers and chairs must disclose if they have such a conflict of interest with a specific submission, and if so, a different chair and/or peer reviewer should be assigned to handle that submission.

To help determine conflicts of interest, and for all other ethical guidelines, we use the Systems and Control Transactions ethical guidelines described at: <https://psecommunity.org/contributor-guidelines>

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Liquid Organic Hydrogen Carriers: comparing alternatives through H₂ equivalent analysis

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ABSTRACT

Liquid Organic Hydrogen Carriers (LOHCs) represent a promising solution for the efficient transport and storage of hydrogen, addressing critical challenges associated with its low volumetric density and safety concerns in gaseous and liquefied forms. LOHCs are oil-like substance, capable of reversibly binding and releasing hydrogen through catalytic hydrogenation and dehydrogenation. Hydrogenation is performed where renewable energy is extensively available: at the loading terminal, green H₂ is produced and is chemically bonded to the LOHC molecule. In this way, the hydrogenated molecule is transported safely under ambient conditions using existing liquid fuels infrastructures. At the delivery site, the dehydrogenation process releases high-purity hydrogen for industrial or mobility applications, with the regenerated LOHC carrier being recycled back to the H₂ production site for reuse. In view of highlighting critical issues associated to LOHCs implementation at large scale, this paper explores green H₂ transport through toluene and dibenzyltoluene. Considering the overall H₂ transport value chain, the performances of these two alternatives are assessed by means of equivalent H₂ methodology. As a result, insights are provided on their role in enabling a sustainable and efficient hydrogen economy.

Keywords: green H₂ transport, LOHC, clean energy, toluene, dibenzyltoluene.

INTRODUCTION

In the transition towards sustainable energy, green hydrogen has gained attention as a low-emission alternative. However, its transport is hindered by its low volumetric density. To address this challenge, various hydrogen carriers have been proposed as a more practical solution. These hydrogen-bearing compounds can be transported more easily at milder conditions and dehydrogenated upon arrival to release hydrogen. Among all the possible options, liquid organic hydrogen carriers (LOHCs) are considered promising due to their compatibility with existing infrastructures [1]. Various LOHCs have been explored in the literature. While some compounds are more suitable for hydrogenation and dehydrogenation, certain criteria help in identifying optimal candidates. The ideal LOHC should have a low melting point and high boiling point to avoid solidification and volatility issues, respectively, a high hydrogen storage capacity, low dehydrogenation enthalpy, low toxicity and be cost-effective at the same time [2].

Once the hydrogen carrier is selected, a detailed techno-economic assessment of the entire H₂ value chain is essential to compare alternatives and demonstrate their feasibility. The H₂ value chain typically includes: hydrogenation of the organic molecule exploiting green H₂, produced where renewable energy sources are extensively available, transport of the hydrogenated compound to its final destination and, upon arrival, dehydrogenation to release hydrogen.

In this framework, the aim of this work is to present a systematic methodology for comparing different H₂ value chains. Toluene (TOL) and dibenzyltoluene (DBT) are selected as representative carriers due to their promising characteristics. A harbor-to-harbor scenario is discussed, to study long distance H₂ transport. The hydrogenation and dehydrogenation stages were designed in Aspen Plus V11®. Based on process simulations, a detailed technical assessment is provided. Each stage of the value chain (*i.e.*, hydrogenation, seaborne transport, dehydrogenation) is technically discussed. Energy consumptions are expressed in terms of equivalent H₂,

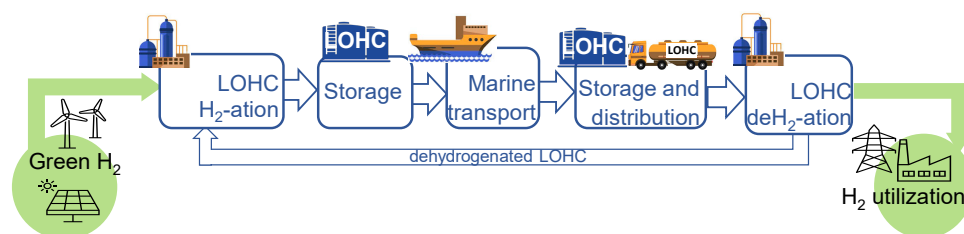


Figure 1: Hydrogen value chain exploiting LOHCs as H₂ carriers.

which, in the end, lowers the amount of hydrogen delivered at the utilization hub. In this way, the efficiency of each stage can be easily quantified. Weaknesses and drawbacks are pointed out, to pave the way for future process intensification.

H₂ TRANSPORT SCENARIO: BASIS OF DESIGN

The H₂ value chain considering LOHCs as H₂ carriers is reported in Figure 1.

A harbor-to-harbor H₂ transport scenario is assumed. At the loading terminal, a flat H₂ production by 100 MW alkaline electrolyzers is considered. These electrolyzers, operating at 20 bar, are responsible for delivering 20000 Nm³/h of H₂. The assumed production scale of the alkaline electrolyzers results in significantly lower H₂ production compared to conventional steam reforming plants. This limitation arises because renewable energy-driven industrial sites must align their scale with the land requirements of renewable energy installations.

At the loading terminal, H₂ is reacted with an organic carrier through an exothermic hydrogenation process and the resulting hydrogenated compound stored before seaborne transport.

The maritime distance between harbours is 2500 km, with the ship powered by traditional fossil-based fuels (IFO 380 1% S).

Upon arrival at the unloading terminal, the hydrogenated carrier is transported to a H₂ valley located 100 km inland via truck.

At the H₂ valley, the carrier undergoes a dehydrogenation reaction to release hydrogen. The released hydrogen meets industrial application standards, being produced at 30 bar with a purity exceeding 99.9 mol%.

The conversion and reconversion stages are the core of the whole hydrogen value chain: for this reason, a detailed technical assessment is performed by means of Aspen Plus V11® process simulations, discussed in the following section. Details about the thermodynamic property package are provided elsewhere [4]. On the other hand, for storage, maritime and road transport, reference is made to the available literature [3]. As the organic carriers are oil-like substances, they are compatible with

existing oil-handling infrastructure, making their integration seamless.

SIMULATION OF THE COST-DRIVING PROCESSES

Hydrogenation section for toluene and dibenzyltoluene are reported in Figure 2.

Referring to toluene hydrogenation section, reported in Figure 2a, toluene, both from the unloading terminal and from make-up stream, enters the process unit's battery limits. It is pressurized and heated to the reaction conditions of 20 bar and 210°C [4]. Reactants pre-heating is performed into a process-to-process heat exchanger (PREHEAT in Figure 2a) to recover the high enthalpy of the reaction products. The hydrogenation reaction (1) is highly exothermic: N₂ acts as a thermal diluent. Its flowrate is such that its concentration in the reactor inlet stream (REAC-IN in Figure 2a) is approximately 17 mol% [5]. Alongside nitrogen and toluene, green hydrogen produced via water electrolysis (stream H₂ in Figure 2a) is also supplied to the battery limits.



The reactor outlet stream (REAC-OUT in Figure 2a), consisting of unreacted hydrogen, nitrogen, and methylcyclohexane, is cooled in the PREHEAT exchanger before proceeding to the separation stages. The separation section, comprising two flash drums in series (FLASH 1 and FLASH 2 in Figure 2a), purifies the reactor output from heavy ends, before and, then, from light ends. The resulting methylcyclohexane (MCH in Figure 2a) is stored and transported by ship to the unloading terminal. Unconverted hydrogen (stream LIGHTEST in Figure 2a) is compressed in COMP and recycled back to the reaction section.

On the other hand, Figure 2b shows the dibenzyltoluene (DBT) hydrogenation process. The organic carrier, HO-DBT in Figure 2b, is sourced from the unloading terminal. Along with a minimal make-up stream, it is routed to the reactor after being pressurized and heated. The reactor (B2 in Figure 2b) is fed with dibenzyltoluene, hydrogen, and nitrogen, with N₂ flow rate set identically to that used in the toluene hydrogenation process.

The reactor, operated at 35 bar and 210°C [6], performs DBT hydrogenation as in reaction (2).



The reaction products, primarily the hydrogenated species, are cooled and stored for transportation to the unloading terminal. In this case, the separation section downstream of the reactor is simplified, as hydrogen conversion is complete and by-product formation during the reaction is negligible. This characteristic is widely recognized in the literature as a key advantage of dibenzyltoluene as a hydrogen carrier [7]. Additionally, DBT's higher molecular weight compared to toluene enables more effective separation based on vapor-liquid equilibrium, as the larger difference in relative volatilities enhances separation efficiency for lighter compounds.

For the sake of comparison between toluene and dibenzyltoluene hydrogenation, Table 1 reports the thermal energy consumptions and Table 2 provides the electric energy consumptions, retrieved from process simulations.

The dehydrogenation process for both methylcyclohexane and perhydro-dibenzyltoluene (H18-DBT) is shown in Figure 3. As for methylcyclohexane (Figure 3a), it enters the process, it is pressurized and directed to the reaction section. The reactor (REACTOR in Figure 3a) operates at 350°C and is responsible for producing toluene and hydrogen according to reaction (3).

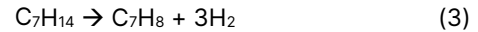


Table 1: Thermal energy consumption for hydrogenation sections of Figure 2. Duty is assumed positive when entering the system.

equipment	T_{in} [°C]	T_{out} [°C]	Q [kW]
<i>toluene hydrogenation</i>			
REACTOR	146	210	-14557.1
COOLER	82	50	-3378.5
<i>dibenzyltoluene dehydrogenation</i>			
COOLER	82.08	50	-482.3
REACTOR	175.11	210	-16462.3

Table 2: Electric energy consumption for hydrogenation sections of Figure 2.

equipment	P_{in} [°C]	P_{out} [°C]	W [kW]
<i>toluene hydrogenation</i>			
PUMP	1.01	20	22.05
COMP	1.01	20	1271
<i>dibenzyltoluene dehydrogenation</i>			
PUMP	1.01	35	47.17
COMPR	20	35	550.6

The reactor's outlet mixture, composed of minor undesired byproducts (primarily benzene), together with

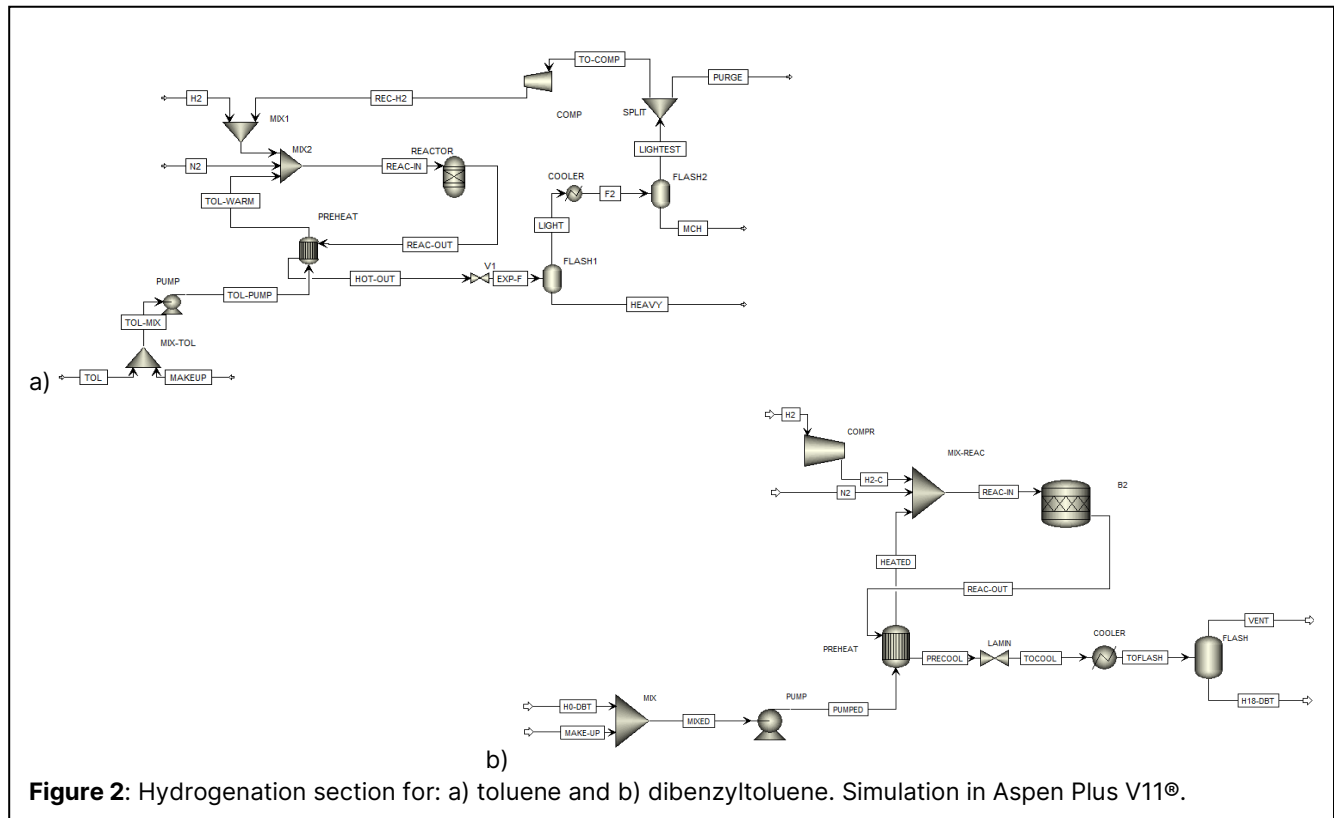


Figure 2: Hydrogenation section for: a) toluene and b) dibenzyltoluene. Simulation in Aspen Plus V11®.

toluene and hydrogen, is sent to the downstream separation train. The separated toluene stream (OUT-TOL in Figure 3a) is stored and subsequently routed back to the loading terminal. Hydrogen is purified via pressure swing adsorption (PSA) to achieve the necessary purity specifications for its intended applications.

The dehydrogenation reaction is highly endothermic, requiring a significant heat supply. This heat is provided by burning a portion of the hydrogen produced, along with waste streams (V and VENT in Figure 3a). As a result of this arrangement, the high endothermicity of the dehydrogenation reaction reduces the net amount of hydrogen available for utilization.

In a similar fashion, Figure 3b shows the process simulation performed for the H18-DBT dehydrogenation. The H18-DBT entering the system is pressurized and directed to the reaction section. The reactor (REACTOR in Figure 3b) operates at 320°C and 1.1 bar. In this unit, H₂ is obtained according to reaction (4).



The reactor's output mixture, consisting of DBT and hydrogen, is processed through a series of separation stages downstream of the reaction section. The recovered DBT (DBT-OUT in Figure 3b) is stored and transported back to the loading terminal, while the hydrogen, which is nearly pure, is compressed and sent to the hydrogen valley for utilization.

Table 3 and Table 4, provide, respectively, the thermal energy consumptions and the electric energy consumptions of the processes depicted in Figure 3.

Table 3: Thermal energy consumption for dehydrogenation sections of Figure 3. Duty is assumed positive when entering the system.

equipment	T_{in} [°C]	T_{out} [°C]	Q [kW]
<i>methylcyclohexane dehydrogenation</i>			
REACTOR	210	350	20093
COOL1	100	50	-3344.6
COOL2	198	80	-996.1
COOL3	240	50	-1943.6
<i>perhydro-dibenzyltoluene dehydrogenation</i>			
REACTOR	306.8	320	19887.3
COOL1	184.8	60	-1002.3
COOL2	235.9	50	-1347.0
COOL3	220.8	50	-1238.5
COOL4	219.9	50	-1234.2

Table 4: Electric energy consumption for dehydrogenation sections of Figure 3.

equipment	P_{in} [°C]	P_{out} [°C]	W [kW]
<i>methylcyclohexane dehydrogenation</i>			
PUMP	1.01	3	2.62
COMP-1	2.9	9.3	1113.3
COMP-2	9.3	30	1231.2
REC-COM	2.9	3	2.17
<i>dibenzyltoluene dehydrogenation</i>			
PUMP	1.01	1.1	0.14
COMP1	1.01	3.15	1148
COMP2	3.15	9.74	1081.5
COMP3	9.74	30	1080.2
COMP-R	1.01	1.1	5.75

To assess the viability of toluene and dibenzyltoluene as H₂ carriers and compare their performances, the equivalent H₂ methodology is applied, which is described in the following section.

TECHNICAL ASSESSMENT: EQUIVALENT H₂ METHODOLOGY

The Equivalent Hydrogen Methodology (EHM) provides a common metric for evaluating the energy content and efficiency of H₂ production, storage and transportation. By calculating the net equivalent hydrogen consumption ($NEHC$) of each energy-consuming process, the Equivalent Hydrogen Methodology enables a more accurate assessment of the total energy required for the full hydrogen cycle, from production to utilization. Then, by subtracting the $NEHC$ to the H₂ entering the process battery limits, the net equivalent H₂ delivered ($NEHD$) to the utilization hub is evaluated, as shown in equation (5).

$$NEHD = F_{H_2,in} - NEHC \quad (5)$$

In this way, this methodology allows to standardize and simplify the comparison of different H₂ carriers, in view of identifying the most cost-effective hydrogen solution.

For the evaluation of $NEHC$, heating above the ambient temperature ($NEHC_{h,i}$), cooling below ambient temperature ($NEHC_{c,i}$) and electric power supply ($NEHC_{e,i}$) are accounted for, thus neglecting heating below ambient temperature (< 25°C) and cooling above ambient temperature (> 25°C) [8] (equation (6)).

$$NEHC = \sum_i NEHC_{h,i} + NEHC_{c,i} + NEHC_{e,i} \quad (6)$$

$$NEHC_{e,i} = \frac{W_i}{\eta_{FC-LHV}} \quad (7)$$

In the present case-study, heating above ambient temperature is achieved by process-process heat exchange, when feasible. Otherwise, heating is provided by either burning part of the hydrogen produced, as in the

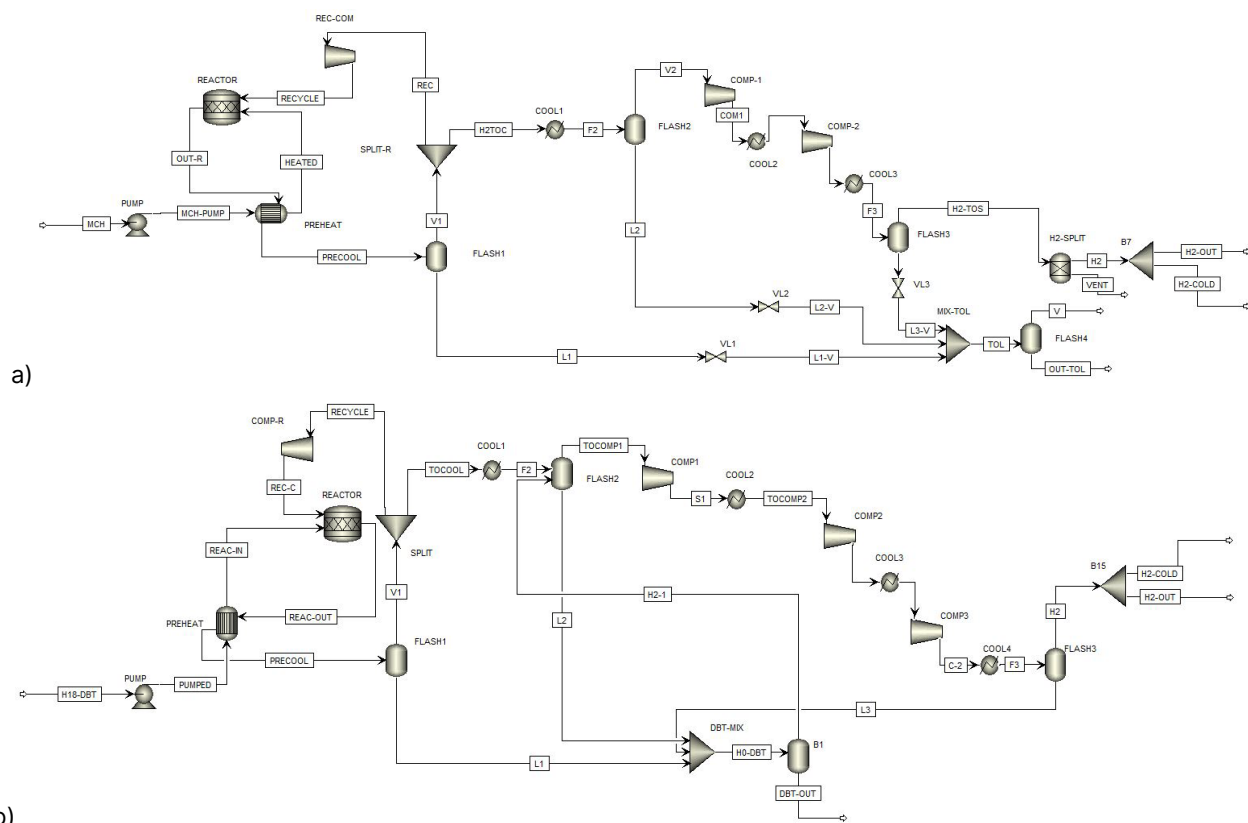


Figure 3: Dehydrogenation section for: a) methylcyclohexane and b) H18-DBT. Simulation in Aspen Plus V11®.

dehydrogenation section. In this case, the term $NEHC_{h,i}$ of equation (6) is retrieved from process simulation [3]. In addition, cooling below the ambient temperature is not required considering the value chain of Figure 1. Finally, the Net Equivalent Hydrogen Consumed for supplying electric power ($NEHC_{e,i}$), used for driving compressors and pumps, is calculated according to equation (7), assuming H_2 utilization in fuel cells with an efficiency (η_{FC}) of 60%. In equation (7), W_i is the electric power consumption retrieved from Aspen Plus V11® simulations, while LHV is the H_2 lower heating value, assumed equal to 120 MJ/kg.

CONCLUSION

Figure 4 summarizes the results of the equivalent H_2 methodology, considering both toluene and dibenzyltoluene as H_2 carriers.

As can be observed from Figure 4, dibenzyltoluene is more effective for H_2 transport than toluene, allowing for a higher H_2 flow rate delivered at the unloading terminal.

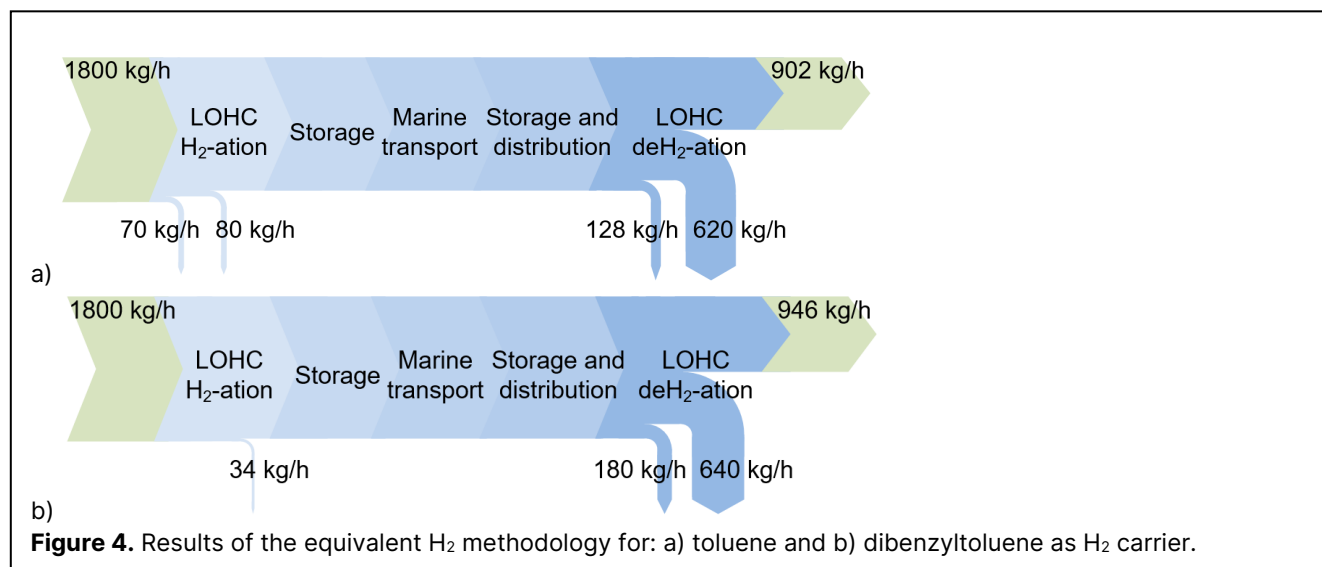
In both cases, part of the green hydrogen entering the battery limits is lost in the hydrogenation stage. The toluene hydrogenation stage is more energy-intensive than the dibenzyltoluene one: this is due to the higher

electric consumption of the hydrogenation stage, because of the H_2 recycle compressor.

As opposite to other H_2 carriers (*i.e.*, liquefied hydrogen or ammonia), no H_2 losses because of the carrier boil off occur during storage and seaborne transport. One of the main advantages of LOHCs is their capability of storing hydrogen without significant degradation or loss over time, making them ideal for balancing seasonal variations in renewable energy supply. In addition, they are stable under ambient temperature and pressure, reducing the risks associated with hydrogen's volatile and explosive nature.

Regarding the dehydrogenation process, the perhydro-dibenzyltoluene dehydrogenation turns out to be less efficient than the methylcyclohexane one. However, for both of the instances analysed, dehydrogenation processes require significant energy input, which reduces the overall efficiency. A non-negligible amount of the H_2 delivered to the unloading terminal is burnt to cope for the endothermicity of the reaction. Moreover, the use of precious metal catalysts (*e.g.*, Pt-based) in hydrogenation and dehydrogenation reactions increases operational costs and catalyst deactivation over time adds to maintenance expenses.

As a result, this assessment confirms that the LOHCs can store significant amounts of hydrogen by



chemically binding it, offering high volumetric hydrogen storage density compared to gaseous or cryogenic hydrogen. The liquid-like nature of LOHCs allows them to be transported using existing fuel distribution and storage infrastructure, including pipelines, tanks, and ships.

The carrier molecules can be regenerated and re-used for multiple cycles of hydrogenation and dehydrogenation, making LOHC systems sustainable over the long term.

On the other hand, their dehydrogenation is highly energy intensive. For this reason, it is essential to identify species with a lower dehydrogenation enthalpy to enhance the dehydrogenation section energy balance. Also, more active and selective catalysts are needed to enable the dehydrogenation at milder operating conditions.

Finally, it must be noted that both of the LOHC molecules involve fossil-derived feedstocks, raising concerns about the overall environmental footprint if not sustainably sourced, despite the closed cycle realised. Future research should be focus on finding suitable carriers derived from renewable feedstocks, improving the life cycle assessment of the whole value chain.

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